

Supporting Information for

Switching the Local Symmetry from D_{5h} to D_{4h} for Single-molecule Magnets by non-Coordinating Solvents

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1. Experimental

1.1 Materials and method

All reactions were carried out under a dry and oxygen-free argon atmosphere in a glovebox. THF, Toluene and Hexane were dried and degassed by standard techniques. Anhydrous DyCl_3 salts were prepared according to the literature procedure, 4-Phenylpyridine (4-PhPy), Na^tOBu and NaBPh_4 are commercially available and were directly used without further treatment.

1.2 Synthesis of the complex 1 and 2

Synthesis of complex $[\text{Dy}^t\text{OBu})_2(4\text{-PhPy})_4][\text{BPh}_4]$ (**1**)

In an argon glovebox, reactants of DyCl_3 (0.5 mmol, 134 mg), Na^tOBu (1 mmol, 96mg) and NaBPh_4 (0.5 mmol, 171 mg) are added into about 10 mL THF in Schlenk tube and gives a cloudy solution, which was filtrated and the solvent was removed by vacuum to get a white powder of the products. And then, add the 2 ml Tol and 4-PhPy (3 mmol, 465 mg) to the powder. In the end, the Crystals suitable for X-ray diffraction were grown by slow diffusion of hexane to THF solution of **1** at room temperature and then obtained the better quality colorless block crystal after three days. Yield 278mg, 36% (based on Dy). Elemental analysis calcd (%) for $\text{C}_{98}\text{H}_{95}\text{BDyN}_5\text{O}_2$: C 76.03, H 6.19, N 4.52; found: C 76.05, H 6.20, N 4.53. IR as showed in Figure S1.

Synthesis of complex $\text{Na}\{[\text{Dy}(\text{O}^t\text{Bu})_2(4\text{-PhPy})_4][\text{BPh}_4]_2\} \cdot 2\text{thf} \cdot \text{hex}$ (**2**)

The synthesis was the same as **1** with THF replaced by Tol, the detailed process can be seen in our previous reported literature^[5].

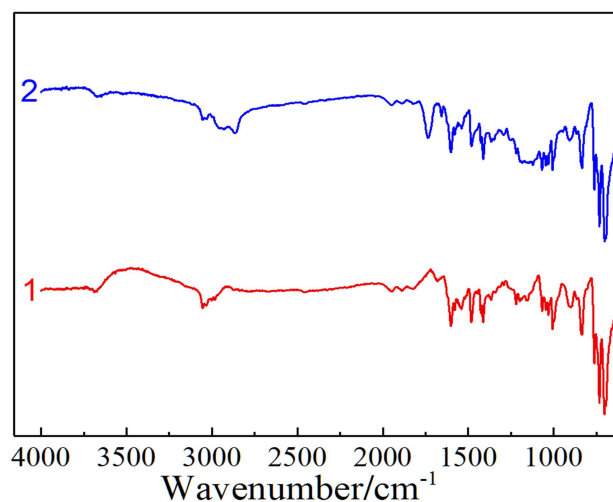


Figure. S1 The IR spectrum of complex **1** and **2**

2. X-ray Crystallography Data

All data were recorded on a Bruker SMART CCD diffractometer with MoK α radiation ($\lambda = 0.71073$ Å). The structures were solved by direct methods and refined on F^2 using SHELXTL. CCDC 2086927 (**1**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge via www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB21EZ, UK; fax: (+44)1223-336-033; or deposit@ccdc.cam.ac.uk).

Table S1. Crystallographic data for complex **1** and **2**.

Complex	1	2
Formula	C ₉₈ H ₉₅ BDyN ₅ O ₂	C ₁₁₄ H ₁₂₄ B ₂ DyN ₄ NaO ₄
F.w.	1548.09	1821.27
T (K)	150	150
Space group	$P-1$	$Pn-3n$
a (Å)	14.573(17)	31.276(5)
b (Å)	15.991(19)	31.276(5)
c (Å)	19.048(2)	31.276(5)
α (°)	91.490(2)	90
β (°)	91.613(2)	90
γ (°)	112.743(2)	90
V (Å ³)	4089.1(8)	30595.6(15)
Z	2	6
D_c (g.cm ⁻³)	1.257	0.593
μ (mm ⁻¹)	0.966	2.180
R_1 ($>2\sigma$ /all data)	0.0370/0.0852	0.0668
wR_2 ($>2\sigma$ /all data)	0.0505/0.0907	0.2063
GOF	1.044	1.050
Residues (e Å ⁻³)	1.53/-1.01	1.49/-0.98
CCDC	2086927	1970693

Table S2. Selected Bond Lengths (Å) and Bond Angles (deg) for complex **1** and **2**.

Complex 1			
Dy(1)-O(1)	2.125(2)	O(1)-Dy(1)-O(2)	175.14(9)
Dy(1)-O(2)	2.121(2)	N(1)-Dy(1)-N(2)	70.60(9)
Dy(1)-N(1)	2.549(3)	N(1)-Dy(1)-N(4)	74.39(9)
Dy(1)-N(2)	2.591(3)	N(3)-Dy(1)-N(4)	75.88(9)
Dy(1)-N(3)	2.585(3)	N(3)-Dy(1)-N(5)	70.43(9)
Dy(1)-N(4)	2.594(3)	O(1)-Dy(1)-N(3)	89.70(9)
Dy(1)-N(5)	2.566(3)	O(2)-Dy(1)-N(4)	89.23(9)
N(1)-C(1)	1.337(6)	O(2)-Dy(1)-N(1)	91.70(9)

Complex 2			
Dy(1)-O(1)	2.066(8)	O(1)-Dy(1)-O(1) ¹	180.0
Dy(1)-O(1) ¹	2.066(8)	O(1) ¹ -Dy(1)-N(1)	90.0 (1)
Dy(1)-N(1)	2.468(6)	O(1)-Dy(1)-N(1) ¹	90.0(2)
Dy(1)-N(1) ¹	2.468(6)	O(1)-Dy(1)-N(1) ²	90.0(3)
Dy(1)-N(1) ²	2.468(6)	O(1)-Dy(1)-N(1) ³	90.0(1)
Dy(1)-N(1) ³	2.468(6)	N(1)-Dy(1)-N(1) ¹	180.0(5)
O(1)-C(8)	1.434(13)	O(1) ¹ -Dy(1)-N(1) ¹	90.0(1)
N(1)-C(1)	1.337(6)	O(1) ¹ -Dy(1)-N(1) ²	90.0(1)
C(1)-C(2)	1.358(6)	N(1)-Dy(1)-N(1) ³	90.0(1)
C(3)-C(4)	1.486(10)	N(1) ¹ -Dy(1)-N(1) ²	90.0(2)
C(5)-C(6)	1.384(8)	N(1) ² -Dy(1)-N(1) ³	90.0(1)
N(1)-Dy(1)-N(1) ²	180.0(5)	N(1) ¹ -Dy(1)-N(1) ³	90.0(1)

¹3/2-X,1/2-Y,+Z; ²3/2-X,+Y,3/2-Z; ³+X,1/2-Y,3/2-Z

Table S3. The CShM's values of the first coordination sphere of compound **1**, referring to all standard 7 vertices polyhedrons.

Reference shapes	HP-7	HPY-7	PBPY-7	COC-7	CTPR-7	JPBPY-7	JETPY-7
Symmetry	D_{7h}	C_{6v}	D_{5h}	D_{3v}	C_{2v}	D_{5h}	C_{3v}
1	33.412	22.977	0.889	7.911	6.022	1.351	23.065

HP-7: Heptagon; HPY-7: Hexagonal pyramid; PBPY-7: Pentagonal bipyramid; COC-7: Capped octahedron; CTPR-7: Capped trigonal prism; JPBPY-7: Johnson pentagonal bipyramid; JETPY-7: Johnson elongated triangular pyramid.

Table S4. The CShM's values of the first coordination sphere of compound **2**, referring to all standard 6 vertices polyhedrons.

Reference Shapes	Hexagon	Pentagonal pyramid	Octahedron	Trigonal prism	Johnson pentagonal pyramid
Symmetry	D_{6h}	C_{5v}	O_h	D_{3h}	C_{5v}
Dy1 in 2	33.216	28.954	0.693	16.800	31.659

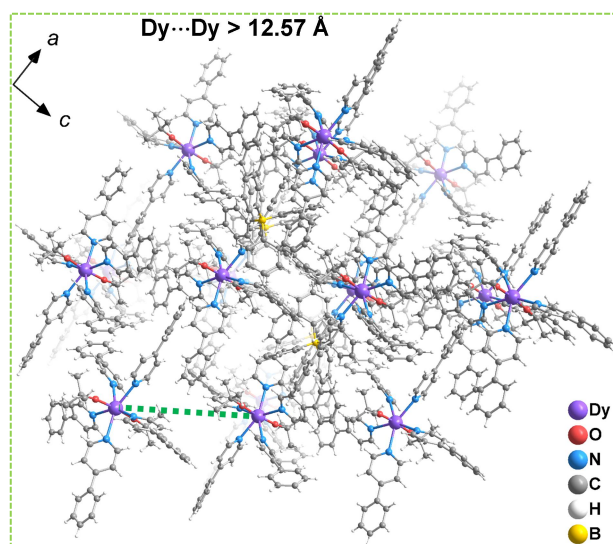


Figure S2. Packing diagram for complex **1**.

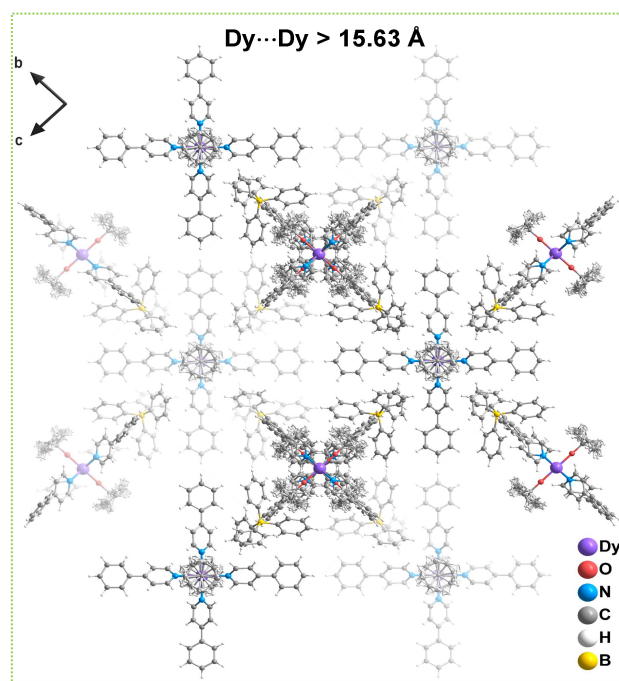


Figure S3. Packing diagram for complex 2.

3. Magnetic Properties

Magnetic susceptibility measurements have been carried out with a Quantum Design MPMS-XL7 SQUID magnetometer upon cooling from 300 to 2 K in variable applied fields. Ac susceptibility measurements have been performed at frequencies of between 1 and 1500 Hz with an oscillating field of 3.5 Oe and with variable dc applied field. Powder samples were embedded in eicosane to avoid any field induced crystal reorientation. Crystalline powders were fixed with eicosane, wrapped with film, and placed in the center of a straw. A diamagnetic correction has been calculated from Pascal constants and embedding eicosane has been applied to the observed magnetic susceptibility.

Table S4. Relaxation fitting parameters of a generalized Debye model for **1**.

T	χ_s	χ_r	τ	α
40	0.03718	0.06511	0.00111	4.04035E-17
43	0.04284	0.11819	0.02832	4.17255E-16
46	0.04156	0.10175	0.00845	7.31436E-16
49	0.04035	0.09102	0.00211	8.90148E-16
52	0.04178	0.08608	7.32758E-4	1.51462E-15
55	0.04719	0.08157	3.41279E-4	2.43371E-15
58	0.06664	0.10137	0.00917	1.37924E-22
61	0.0669	0.13069	0.07542	4.34904E-22
64	0.0643	0.1246	0.06952	6.25656E-22
67	0.06114	0.11987	0.05657	1.28719E-21
70	0.0596	0.11461	0.04454	1.9819E-21
73	0.05721	0.1098	0.03006	3.28085E-21
76	0.05424	0.10693	0.01862	4.75149E-21
79	0.05315	0.1036	0.0099	8.60968E-21
82	0.05076	0.09957	0.00506	1.52023E-20
85	0.04903	0.09574	0.00265	2.93391E-20
88	0.04733	0.09199	0.00134	5.62355E-20
91	0.04736	0.09009	7.3934E-4	8.59742E-20
94	0.04476	0.08729	3.8823E-4	1.39697E-19
97	0.04422	0.08469	2.30956E-4	1.68881E-19

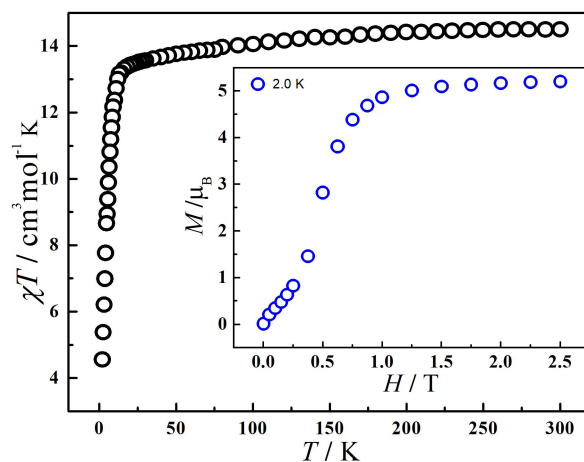


Figure S4. The variable-temperature dc magnetic susceptibility (1000 Oe) and the field dependence of the magnetization (inset) at 2 K for **1**.

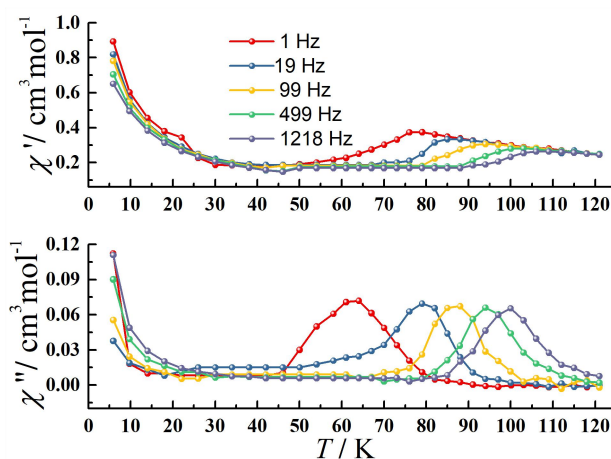


Figure S5. Temperature-dependence of the in-phase (χ') and out-of-phase (χ'') ac susceptibility signals under zero dc field for **1**.

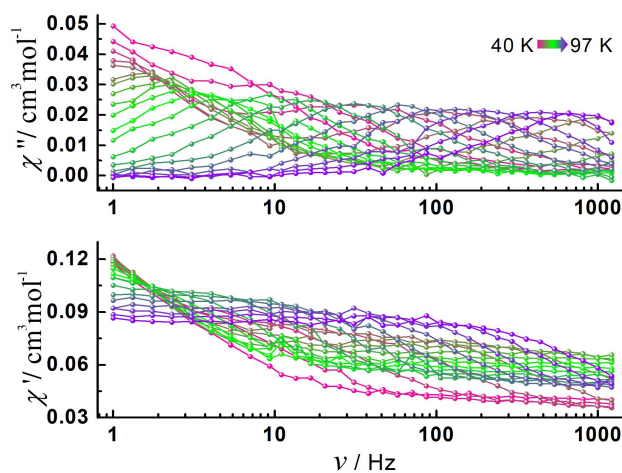


Figure S6. Frequency-dependence of the in-phase χ' and out-of-phase χ'' in a zero dc field for **1** with ac frequencies of 1-1218 Hz.

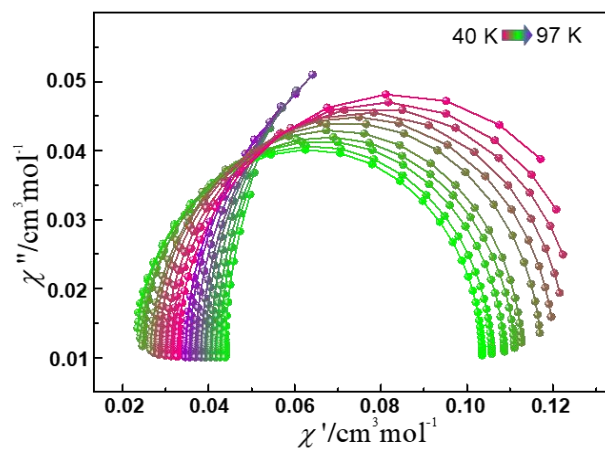


Figure S7. Cole-Cole plots for the ac susceptibilities in a zero dc field for **1**. The solid lines are the best fit to Debye's law.

4. Electronic Structure Calculations

Complete Active Space Self-consistent Field (CASSCF) calculation was performed to understand magnetic properties of **1** via its electronic structure using OPEN MOLCAS^[1] and its geometry structure was obtained straightly from X-Ray single crystal structure without optimization. The basis sets from the ANO-RCC library^[2] were employed for all atoms: VTZP quality for Dy, VDZP quality for O and N atoms as well as VDZ quality for others. 21 sextets, 224 quartets and 490 doublets were calculated in RASSCF module to acquire the state-averaged CASSCF orbitals. Then spin-orbit (SO) coupling Hamiltonian was constructed and diagonalized in RASSI module^[3] through chosen 21 sextets, 128 quartets and 130 doublets. Ultimately all magnetic properties of Dy(III) ion, such as *g*-tensors, crystal field parameters, transition magnetic moment matrix, magnetic susceptibility and magnetization plot, were computed and output via SINGLE_ANISO program^[4]. For assuring calculation accuracy, we also considered employing the Cholesky decomposition for two-electron integrals.

Table S5 *Ab initio* results for the $J = 15/2$ multiple of Dy^{III} in **1**.

Energy (cm ⁻¹)	Energy (K)	<i>g_x</i>	<i>g_y</i>	<i>g_z</i>	<i>g_z</i> Angle (°)	Crystal field Wavefunction
0	0	0.00	0.00	19.89	-	99.9% ±15/2>
543	781	0.00	0.00	16.98	1.32	99.8% ±13/2>
904	1300	0.09	0.11	14.26	3.42	99.4% ±11/2>
1096	1576	0.81	1.96	10.58	10.85	87.1% ±9/2>
1138	1636	1.44	4.98	12.96	86.86	70.1% ±1/2>
1155	1660	0.99	3.61	7.49	88.78	16.5% ±3/2>+41.0% ∓3/2>+21.8% ∓7/2>
1186	1705	3.26	4.01	13.71	87.84	11.6% ±5/2>+ 22.2% ∓3/2>+35.7% ∓7/2>
1195	1718	1.18	5.61	12.36	82.40	54.1% ±5/2> +23.3% ∓7/2>

*Only components with > 10% contribution are given, rounded to the nearest percent.

Table S6 *Ab initio* calculated crystal field parameters for **1**.

Crystal Field Parameter(B_q^k)		Value / cm^{-1}	Crystal Field Parameter(B_q^k)		Value / cm^{-1}
q	k		q	k	
2	-2	0.16860990836356E-01	6	-6	-0.31084107978718E-04
2	-1	-0.19680699199121E-01	6	-5	-0.16901297741972E-04
2	0	-0.65300508096316E+01	6	-4	0.33265651601129E-04
2	1	0.90487472385106E-02	6	-3	-0.34879042563356E-04
2	2	0.40649055336602E+00	6	-2	0.26612047507683E-05
4	-4	0.43943620276023E-02	6	-1	0.29672991397177E-04
4	-3	-0.55323343438564E-02	6	0	0.13229739082706E-04
4	-2	-0.20422541516122E-03	6	1	-0.17214006060346E-04
4	-1	0.45422261591697E-02	6	2	0.30193690203995E-05
4	0	-0.13955624451093E-01	6	3	-0.30863681029782E-04
4	1	-0.17384774314924E-02	6	4	0.24365214177074E-04
4	2	0.80087584394893E-03	6	5	-0.19712406667379E-03
4	3	-0.57855134523574E-02	6	6	-0.88795517281251E-04
4	4	0.40687627009409E-02			

Table S7 *Ab initio* calculated LoProp charges of the atoms near Dy center in **1**.

Dy	O ₁	O ₂	N ₁	N ₂	N ₃	N ₄	N ₅
2.4385	-1.0467	-1.0664	-0.3639	-0.3559	-0.3656	-0.3592	-0.3584

Table S8 Average transition magnetic moment elements between the states of **1**, given in μ_B^2 .

	$ +\frac{15}{2}\rangle$	$ -\frac{15}{2}\rangle$	$ +\frac{13}{2}\rangle$	$ -\frac{13}{2}\rangle$	$ +\frac{11}{2}\rangle$	$ -\frac{11}{2}\rangle$	$ +\frac{9}{2}\rangle$	$ -\frac{9}{2}\rangle$	$ +a\rangle$	$ -a\rangle$	$ +b\rangle$	$ -b\rangle$	$ +c\rangle$	$ -c\rangle$	$ +d\rangle$	$ -d\rangle$
$ +\frac{15}{2}\rangle$		1.5E-10	4.4E+00	3.4E-07	4.3E-03	1.2E-06	8.9E-04	1.1E-05	1.7E-04	1.7E-05	3.1E-04	3.9E-05	1.6E-04	2.5E-05	1.1E-04	1.5E-04
$ -\frac{15}{2}\rangle$	1.5E-10		3.4E-07	4.4E+00	1.2E-06	4.3E-03	1.1E-05	8.9E-04	1.7E-05	1.7E-04	3.9E-05	3.1E-04	2.5E-05	1.6E-04	1.5E-04	1.1E-04
$ +\frac{13}{2}\rangle$	4.4E+00	3.4E-07		9.8E-06	8.3E+00	3.5E-04	1.1E-02	2.0E-03	3.4E-03	5.0E-03	3.3E-03	9.5E-04	2.4E-03	1.5E-04	1.2E-03	2.7E-03
$ -\frac{13}{2}\rangle$	3.4E-07	4.4E+00	9.8E-06		3.5E-04	8.3E+00	2.0E-03	1.1E-02	5.0E-03	3.4E-03	9.5E-04	3.3E-03	1.5E-04	2.4E-03	2.7E-03	1.2E-03
$ +\frac{11}{2}\rangle$	4.3E-03	1.2E-06	8.3E+00	3.5E-04		4.6E-03	1.1E+01	1.6E-01	2.9E-01	1.7E-01	6.3E-02	2.2E-01	3.0E-02	3.2E-03	1.5E-02	4.3E-02
$ -\frac{11}{2}\rangle$	1.2E-06	4.3E-03	3.5E-04	8.3E+00	4.6E-03		1.6E-01	1.1E+01	1.7E-01	2.9E-01	2.2E-01	6.3E-02	3.2E-03	3.0E-02	4.3E-02	1.5E-02
$ +\frac{9}{2}\rangle$	8.9E-04	1.1E-05	1.1E-02	2.0E-03	1.1E+01	1.6E-01		8.9E-01	1.4E+00	2.7E+00	5.8E+00	9.9E-01	3.6E+00	5.6E-01	1.5E+00	3.8E-01
$ -\frac{9}{2}\rangle$	1.1E-05	8.9E-04	2.0E-03	1.1E-02	1.6E-01	1.1E+01	8.9E-01		2.7E+00	1.4E+00	9.9E-01	5.8E+00	5.6E-01	3.6E+00	3.8E-01	1.5E+00
$ +a\rangle$	1.7E-04	1.7E-05	3.4E-03	5.0E-03	2.9E-01	1.7E-01	1.4E+00	2.7E+00		1.4E+01	1.1E+01	2.8E+00	1.3E+00	8.5E-01	5.2E-01	5.0E-01
$ -a\rangle$	1.7E-05	1.7E-04	5.0E-03	3.4E-03	1.7E-01	2.9E-01	2.7E+00	1.4E+00	1.4E+01		2.8E+00	1.1E+01	8.5E-01	1.3E+00	5.0E-01	5.2E-01
$ +b\rangle$	3.1E-04	3.9E-05	3.3E-03	9.5E-04	6.3E-02	2.2E-01	5.8E+00	9.9E-01	1.1E+01	2.8E+00		5.2E+00	1.2E+00	1.4E+00	2.1E+00	6.6E+00
$ -b\rangle$	3.9E-05	3.1E-04	9.5E-04	3.3E-03	2.2E-01	6.3E-02	9.9E-01	5.8E+00	2.8E+00	1.1E+01	5.2E+00		1.4E+00	1.2E+00	6.6E+00	2.1E+00
$ +c\rangle$	1.6E-04	2.5E-05	2.4E-03	1.5E-04	3.0E-02	3.2E-03	3.6E+00	5.6E-01	1.3E+00	8.5E-01	1.2E+00	1.4E+00		1.3E+01	5.3E+00	5.8E+00
$ -c\rangle$	2.5E-05	1.6E-04	1.5E-04	2.4E-03	3.2E-03	3.0E-02	5.6E-01	3.6E+00	8.5E-01	1.3E+00	1.4E+00	1.2E+00	1.3E+01		5.8E+00	5.3E+00
$ +d\rangle$	1.1E-04	1.5E-04	1.2E-03	2.7E-03	1.5E-02	4.3E-02	1.5E+00	3.8E-01	5.2E-01	5.0E-01	2.1E+00	6.6E+00	5.3E+00	5.8E+00		9.3E+00
$ -d\rangle$	1.5E-04	1.1E-04	2.7E-03	1.2E-03	4.3E-02	1.5E-02	3.8E-01	1.5E+00	5.0E-01	5.2E-01	6.6E+00	2.1E+00	5.8E+00	5.3E+00	9.3E+00	

5. DFT calculations

To acquire wave function information of both complexes and electrostatic potentials (ESP) of distinctive solvents and transversal ligand, the calculations based on Density Function Theory (DFT) were performed using Gaussian 09D^[5]. The PBE density functional^[6,7] was employed in all calculations with Grimme's D3 dispersion correction considered^[8-10]. Primarily, the positions of hydrogen atoms of **1** and **2** were optimized. We replaced Dy(III) ion to Y(III) in light of similar radius between them, and set its atomic mass as 162.5 (the same as natural abundance-weighted mass of dysprosium). The Stuttgart RSC 1997 effective core potential (ECP)^[11,12] was applied for 28 core electrons of Y(III) and corresponding valence basis set was used for the remaining valence electrons, while the rest of atoms were treated with cc-pVDZ^[13,14] basis set. Then the whole molecules of toluene, THF and 4-phenylpyridine were optimized by the same basis set. Harmonic vibrational calculations indicate that there is no imaginary vibration mode and all optimized minimum-energy structures have already been at stationary points on the potential energy surface.

Table S9 Geometry coordinates of **1** in population analysis calculations.

Dy	-0.2003	0.0679	0.1465
O	-0.1715	-0.0710	-1.9740
O	-0.2583	0.0290	2.2664
N	-2.6313	0.8246	0.0185
N	-0.2931	2.6553	0.0679
N	1.5577	-1.8218	0.2805
N	-1.6081	-2.1099	0.1026
N	2.1568	1.0781	0.0501
C	-0.2378	-0.1831	-3.3222
C	-0.3136	-0.1592	3.6421
C	-3.1295	1.3290	-1.1140
C	-3.5060	0.5786	0.9951
C	0.2699	3.3674	-0.9283
C	-0.8147	3.3708	1.0775
C	1.7123	-2.7127	-0.7112
C	2.5522	-1.7674	1.1847
C	-1.3031	-3.1632	0.8729
C	-2.7143	-2.2382	-0.6451
C	2.8399	0.9495	-1.0961
C	2.8561	1.4773	1.1272
C	-0.1420	1.2019	-3.9560
C	0.9166	-1.0482	-3.8644
C	-1.5605	-0.8552	-3.7606
C	0.6830	0.8084	4.2817
C	0.0624	-1.5815	4.0119
C	-1.7173	0.1295	4.1618
C	-4.4666	1.5733	-1.3296
C	-4.8654	0.8124	0.8662
C	0.3519	4.7433	-0.9379
C	-0.7778	4.7492	1.1392
C	2.8191	-3.5042	-0.8676
C	3.7021	-2.5186	1.0979

C	-2.0505	-4.3271	0.9287
C	-3.5247	-3.3448	-0.6431
C	4.1913	1.1546	-1.2057
C	4.2254	1.6602	1.1110
C	-5.3869	1.3204	-0.3138
C	-0.1708	5.4823	0.1189
C	3.8770	-3.4029	0.0333
C	-3.2108	-4.4256	0.1720
C	4.9374	1.4692	-0.0719
C	-6.8377	1.5388	-0.4821
C	-0.0499	6.9626	0.1701
C	5.1306	-4.1866	-0.1175
C	-4.0664	-5.6413	0.2081
C	6.4099	1.5074	-0.1508
C	-7.6441	1.8911	0.6109
C	-7.4495	1.3746	-1.7355
C	1.0051	7.5968	-0.4686
C	-0.9250	7.7338	0.9134
C	5.1130	-5.4905	-0.5713
C	6.3587	-3.6052	0.1824
C	-3.5031	-6.9158	0.2171
C	-5.4560	-5.5241	0.2474
C	7.0679	2.1989	-1.1494
C	7.1689	0.7136	0.7162
C	-9.0140	2.0210	0.4582
C	-8.8160	1.5288	-1.8656
C	1.1579	8.9818	-0.3652
C	-0.7475	9.1003	1.0196
C	6.2919	-6.2119	-0.6806
C	7.5324	-4.3500	0.0560
C	-4.3158	-8.0363	0.2263
C	-6.2484	-6.6466	0.2815
C	8.4422	2.1285	-1.2904
C	8.5370	0.6165	0.5420
C	-9.6004	1.8399	-0.7691
C	0.2827	9.7189	0.3870
C	7.4863	-5.6454	-0.3704
C	-5.6887	-7.9042	0.2721
C	9.1662	1.3241	-0.4456
H	-7.1855	2.0670	1.5947
H	-6.8452	1.0854	-2.6076
H	1.7457	7.0170	-1.0369
H	-1.7829	7.2639	1.4161
H	4.1553	-5.9778	-0.8075
H	6.4112	-2.5533	0.5003
H	-2.4098	-7.0305	0.1721
H	-5.9160	-4.5247	0.2694
H	6.4845	2.8303	-1.8378
H	6.6660	0.1357	1.5066
H	-9.6291	2.2892	1.3297
H	-9.2842	1.3846	-2.8504
H	2.0019	9.4677	-0.8760
H	-1.4614	9.6854	1.6181
H	6.2462	-7.2563	-1.0232
H	8.4952	-3.8733	0.2921

H	-3.8583	-9.0363	0.2074
H	-7.3420	-6.5344	0.3253
H	8.9414	2.7056	-2.0815
H	9.1206	-0.0308	1.2135
H	-10.6885	1.9468	-0.8853
H	0.4155	10.8073	0.4758
H	8.4151	-6.2277	-0.4633
H	-6.3299	-8.7971	0.2927
H	10.2572	1.2453	-0.5644
H	-2.3889	1.5381	-1.9006
H	-3.0886	0.1585	1.9209
H	0.6722	2.7773	-1.7639
H	-1.2684	2.7824	1.8908
H	0.8857	-2.7535	-1.4361
H	2.3992	-1.0634	2.0153
H	-0.3982	-3.0554	1.4880
H	-2.9502	-1.3868	-1.2982
H	2.2377	0.6224	-1.9574
H	2.2733	1.6150	2.0509
H	-0.9449	1.8652	-3.5716
H	-0.2262	1.1740	-5.0618
H	0.8321	1.6746	-3.7083
H	1.9008	-0.6425	-3.5515
H	0.9097	-1.1011	-4.9721
H	0.8409	-2.0847	-3.4786
H	-1.6339	-1.8692	-3.3182
H	-1.6300	-0.9547	-4.8629
H	-2.4341	-0.2646	-3.4163
H	0.6706	0.7685	5.3908
H	1.7148	0.5666	3.9512
H	0.4575	1.8492	3.9702
H	0.0711	-1.7336	5.1110
H	-0.6632	-2.3013	3.5816
H	1.0695	-1.8408	3.6283
H	-1.7777	0.0483	5.2663
H	-2.0373	1.1533	3.8772
H	-2.4422	-0.5953	3.7359
H	-4.7862	1.9990	-2.2906
H	-5.5263	0.5575	1.7063
H	0.8123	5.2402	-1.8025
H	-1.1955	5.2522	2.0218
H	2.8829	-4.1797	-1.7323
H	4.4716	-2.4224	1.8764
H	-1.7426	-5.1389	1.6019
H	-4.4070	-3.3731	-1.2973
H	4.6906	0.9946	-2.1719
H	4.7467	1.9517	2.0342

Table S10 Geometry coordinates of **2** in population analysis calculations.

Dy	0.0066	-0.0001	-0.0001
O	0.0066	0.0088	2.0642
O	0.0066	-0.0107	-2.0629

N	0.0071	2.4666	-0.0110
N	2.4741	-0.0015	0.0006
N	-2.4610	-0.0003	0.0006
N	0.0060	-2.4684	0.0123
C	0.0066	0.0175	3.4985
C	0.0066	-0.0156	-3.4997
C	0.7592	3.1970	0.8203
C	-0.7446	3.1895	-0.8518
C	3.1991	0.7481	-0.8403
C	3.1988	-0.7477	0.8390
C	-3.1860	-0.7541	-0.8332
C	-3.1856	0.7575	0.8319
C	-0.7461	-3.1873	0.8505
C	0.7577	-3.1955	-0.8217
C	0.1203	1.5245	3.8280
C	1.1497	-0.7978	4.0641
C	-1.4028	-0.2343	4.0615
C	0.1195	-1.5245	-3.8280
C	1.1501	0.7973	-4.0642
C	-1.4027	0.2349	-4.0615
H	1.3706	2.6212	1.5313
C	0.8054	4.5541	0.8222
H	-1.3464	2.6038	-1.5665
C	-0.7901	4.5465	-0.8652
H	2.6176	1.3514	-1.5553
C	4.5570	0.7927	-0.8475
H	2.6181	-1.3512	1.5549
C	4.5567	-0.7948	0.8475
H	-2.6047	-1.3684	-1.5395
C	-4.5439	-0.8007	-0.8400
H	-2.6039	1.3723	1.5373
C	-4.5436	0.8028	0.8400
H	-1.3481	-2.6016	1.5650
C	-0.7923	-4.5461	0.8652
H	1.3686	-2.6192	-1.5325
C	0.8032	-4.5544	-0.8223
H	1.1105	1.9282	3.5231
H	-0.6600	2.0794	3.2752
H	0.0065	1.7400	4.9117
H	1.0629	-1.8614	3.7572
H	2.1139	-0.4017	3.6890
H	1.1697	-0.7623	5.1724
H	-1.7710	-1.2634	3.8458
H	-1.4220	-0.1039	5.1616
H	-2.1187	0.4753	3.6099
H	1.1099	-1.9279	-3.5234
H	-0.6606	-2.0782	-3.2740
H	0.0050	-1.7410	-4.9115
H	1.0652	1.8612	-3.7579
H	2.1137	0.3999	-3.6889
H	1.1702	0.7615	-5.1724
H	-1.7719	1.2638	-3.8460
H	-1.4220	0.1046	-5.1616
H	-2.1179	-0.4751	-3.6098
H	1.4583	5.0592	1.5481

C	0.0078	5.2769	-0.0243
H	-1.4402	5.0464	-1.5973
H	5.0605	1.4410	-1.5788
C	5.2844	-0.0021	0.0006
H	5.0581	-1.4437	1.5796
H	-5.0467	-1.4551	-1.5662
C	-5.2713	0.0003	0.0006
H	-5.0462	1.4589	1.5648
H	-1.4436	-5.0444	1.5973
C	0.0053	-5.2787	0.0256
H	1.4551	-5.0601	-1.5487
C	0.0081	6.7635	-0.0326
C	6.7693	-0.0007	-0.0007
C	-6.7561	0.0024	-0.0007
C	0.0050	-6.7618	0.0313
C	-1.1485	7.4624	-0.2777
C	1.1651	7.4641	0.2072
C	7.4696	-1.1574	0.2479
C	7.4701	1.1539	-0.2479
C	-7.4565	1.1597	0.2370
C	-7.4570	-1.1562	-0.2370
C	1.1616	-7.4646	-0.2072
C	-1.1520	-7.4618	0.2777
H	-2.0935	6.9249	-0.4478
C	-1.1454	8.8438	-0.2606
H	2.1095	6.9276	0.3833
C	1.1627	8.8453	0.1784
H	6.9319	-2.1009	0.4255
C	8.8518	-1.1560	0.2256
H	6.9344	2.0986	-0.4250
C	8.8524	1.1500	-0.2243
H	-6.9202	2.1055	0.4060
C	-8.8387	1.1563	0.2147
H	-6.9200	-2.1019	-0.4046
C	-8.8393	-1.1539	-0.2134
H	2.1069	-6.9292	-0.3822
C	1.1586	-8.8477	-0.1771
H	-2.0968	-6.9241	0.4485
C	-1.1496	-8.8451	0.2619
H	-2.0851	9.3884	-0.4327
C	0.0088	9.5118	-0.0456
H	2.1024	9.3911	0.3460
H	9.3973	-2.0946	0.4000
C	9.5176	-0.0013	-0.0007
H	9.3977	2.0889	-0.3983
H	-9.3836	2.0968	0.3805
C	-9.5045	0.0032	-0.0007
H	-9.3850	-2.0941	-0.3783
H	2.0979	-9.3942	-0.3440
C	0.0043	-9.5100	0.0443
H	-2.0890	-9.3896	0.4346
H	0.0091	10.6129	-0.0511
H	10.6188	-0.0015	-0.0009
H	-10.6057	0.0036	-0.0010
H	0.0040	-10.6113	0.0492

Table S11 Geometry coordinates of toluene molecule in population analysis calculations.

C	-1.9137	-0.0051	-0.0003
C	-1.1999	-1.2148	-0.0001
C	0.2014	-1.2063	0.0004
C	0.9211	0.0068	0.0005
C	0.1923	1.2113	0.0004
C	-1.2116	1.2086	-0.0001
H	-3.0133	-0.0104	-0.0006
H	-1.7404	-2.1730	0.0000
H	0.7526	-2.1597	0.0007
H	0.7368	2.1683	0.0007
H	-1.7590	2.1628	0.0000
C	2.4302	0.0035	-0.0003
H	2.8329	-0.5332	0.8837
H	2.8317	-0.5109	-0.8983
H	2.8399	1.0317	0.0119

Table S12 Geometry coordinates of THF molecule in population analysis calculations.

C	1.1255	-0.4722	-0.1672
O	-0.0013	-1.2069	0.3106
C	-1.1278	-0.4692	-0.1634
C	-0.7752	1.0195	0.0510
C	0.7790	1.0160	0.0560
H	2.0167	-0.8211	0.3892
H	1.2887	-0.6742	-1.2563
H	-1.2982	-0.6752	-1.2505
H	-2.0171	-0.8126	0.3995
H	-1.2003	1.6616	-0.7449
H	-1.1703	1.3817	1.0200
H	1.2126	1.6630	-0.7314
H	1.1690	1.3675	1.0310

Table S13 Geometry coordinates of 4-phenylpyridine in population analysis calculations.

C	2.8869	1.0855	0.3557
C	1.4870	1.1398	0.3739
C	0.7439	0.0000	0.0000
C	1.4870	-1.1398	-0.3739
C	2.8869	-1.0855	-0.3557
N	3.6029	0.0000	0.0000
H	3.4736	1.9715	0.6529
H	0.9766	2.0561	0.7040
H	0.9766	-2.0561	-0.7040
H	3.4736	-1.9715	-0.6529
C	-0.7387	0.0000	0.0000
C	-1.4622	-1.1610	0.3523
C	-1.4622	1.1610	-0.3523
C	-2.8631	-1.1600	0.3546
H	-0.9166	-2.0661	0.6559
C	-2.8631	1.1600	-0.3546

H	-0.9166	2.0661	-0.6559
C	-3.5695	0.0000	0.0000
H	-3.4077	-2.0708	0.6429
H	-3.4077	2.0708	-0.6429
H	-4.6690	0.0000	0.0000

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